

David Fairen-Jimenez

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The third column is the impact factor (IF) of the journal, and the fourth column is the number of citations of the article.

116 papers	7,701 citations	45 h-index	86 g-index
131 ext. papers	9,242 ext. citations	9.3 avg, IF	6.25 L-index

#	Paper	IF	Citations
116	Opening the gate: framework flexibility in ZIF-8 explored by experiments and simulations. <i>Journal of the American Chemical Society</i> , 2011 , 133, 8900-2	16.4	773
115	Vapor-phase metalation by atomic layer deposition in a metal-organic framework. <i>Journal of the American Chemical Society</i> , 2013 , 135, 10294-7	16.4	659
114	Development of a Cambridge Structural Database Subset: A Collection of Metal-Organic Frameworks for Past, Present, and Future. <i>Chemistry of Materials</i> , 2017 , 29, 2618-2625	9.6	499
113	A sol-gel monolithic metal-organic framework with enhanced methane uptake. <i>Nature Materials</i> , 2018 , 17, 174-179	27	257
112	Amorphous metal-organic frameworks for drug delivery. <i>Chemical Communications</i> , 2015 , 51, 13878-81	5.8	247
111	Temperature Treatment of Highly Porous Zirconium-Containing Metal-Organic Frameworks Extends Drug Delivery Release. <i>Journal of the American Chemical Society</i> , 2017 , 139, 7522-7532	16.4	216
110	Incorporation of an A1/A2-difunctionalized pillar[5]arene into a metal-organic framework. <i>Journal of the American Chemical Society</i> , 2012 , 134, 17436-9	16.4	209
109	Metal-Organic Framework Thin Films Composed of Free-Standing Acicular Nanorods Exhibiting Reversible Electrochromism. <i>Chemistry of Materials</i> , 2013 , 25, 5012-5017	9.6	194
108	Selective Surface PEGylation of UiO-66 Nanoparticles for Enhanced Stability, Cell Uptake, and pH-Responsive Drug Delivery. <i>Chem</i> , 2017 , 2, 561-578	16.2	183
107	Screening of bio-compatible metal-organic frameworks as potential drug carriers using Monte Carlo simulations. <i>Journal of Materials Chemistry B</i> , 2014 , 2, 766-774	7.3	171
106	Metal-Organic Nanosheets Formed via Defect-Mediated Transformation of a Hafnium Metal-Organic Framework. <i>Journal of the American Chemical Society</i> , 2017 , 139, 5397-5404	16.4	165
105	Elucidating the breathing of the metal-organic framework MIL-53(Sc) with ab initio molecular dynamics simulations and in situ X-ray powder diffraction experiments. <i>Journal of the American Chemical Society</i> , 2013 , 135, 15763-73	16.4	154
104	Flexibility and swing effect on the adsorption of energy-related gases on ZIF-8: combined experimental and simulation study. <i>Dalton Transactions</i> , 2012 , 41, 10752-62	4.3	150
103	Water-stable zirconium-based metal-organic framework material with high-surface area and gas-storage capacities. <i>Chemistry - A European Journal</i> , 2014 , 20, 12389-93	4.8	124
102	Control over Catenation in Pillared Paddlewheel Metal-Organic Framework Materials via Solvent-Assisted Linker Exchange. <i>Chemistry of Materials</i> , 2013 , 25, 739-744	9.6	120
101	Methane storage mechanism in the metal-organic framework Cu ₃ (btc) ₂ : An in situ neutron diffraction study. <i>Microporous and Mesoporous Materials</i> , 2010 , 136, 50-58	5.3	117
100	Metal-organic frameworks as biosensors for luminescence-based detection and imaging. <i>Interface Focus</i> , 2016 , 6, 20160027	3.9	109

99	Tuning porosity in macroscopic monolithic metal-organic frameworks for exceptional natural gas storage. <i>Nature Communications</i> , 2019 , 10, 2345	17.4	100
98	Computer-aided discovery of a metal-organic framework with superior oxygen uptake. <i>Nature Communications</i> , 2018 , 9, 1378	17.4	100
97	Drug delivery and controlled release from biocompatible metal-organic frameworks using mechanical amorphization. <i>Journal of Materials Chemistry B</i> , 2016 , 4, 7697-7707	7.3	100
96	Granular and monolithic activated carbons from KOH-activation of olive stones. <i>Microporous and Mesoporous Materials</i> , 2006 , 92, 64-70	5.3	100
95	Structure-Mechanical Stability Relations of Metal-Organic Frameworks via Machine Learning. <i>Matter</i> , 2019 , 1, 219-234	12.7	99
94	A mechanochemical strategy for IRMOF assembly based on pre-designed oxo-zinc precursors. <i>Chemical Communications</i> , 2015 , 51, 4032-5	5.8	94
93	Porosity and surface area of monolithic carbon aerogels prepared using alkaline carbonates and organic acids as polymerization catalysts. <i>Carbon</i> , 2006 , 44, 2301-2307	10.4	89
92	A novel structural form of MIL-53 observed for the scandium analogue and its response to temperature variation and CO ₂ adsorption. <i>Dalton Transactions</i> , 2012 , 41, 3937-41	4.3	87
91	Shaping the Future of Fuel: Monolithic Metal-Organic Frameworks for High-Density Gas Storage. <i>Journal of the American Chemical Society</i> , 2020 , 142, 8541-8549	16.4	82
90	Noble Gas Adsorption in Copper Trimesate, HKUST-1: An Experimental and Computational Study. <i>Journal of Physical Chemistry C</i> , 2013 , 117, 20116-20126	3.8	80
89	Gate-opening effect in ZIF-8: the first experimental proof using inelastic neutron scattering. <i>Chemical Communications</i> , 2016 , 52, 3639-42	5.8	77
88	High-Throughput Screening of Porous Crystalline Materials for Hydrogen Storage Capacity near Room Temperature. <i>Journal of Physical Chemistry C</i> , 2014 , 118, 5383-5389	3.8	74
87	Core-Shell Gold Nanorod@Zirconium-Based Metal-Organic Framework Composites as in Situ Size-Selective Raman Probes. <i>Journal of the American Chemical Society</i> , 2019 , 141, 3893-3900	16.4	73
86	A general approach for hysteresis-free, operationally stable metal halide perovskite field-effect transistors. <i>Science Advances</i> , 2020 , 6, eaaz4948	14.3	73
85	Efficient identification of hydrophobic MOFs: application in the capture of toxic industrial chemicals. <i>Journal of Materials Chemistry A</i> , 2016 , 4, 529-536	13	71
84	Mechanically and chemically robust ZIF-8 monoliths with high volumetric adsorption capacity. <i>Journal of Materials Chemistry A</i> , 2015 , 3, 2999-3005	13	71
83	Surface-Functionalization of Zr-Fumarate MOF for Selective Cytotoxicity and Immune System Compatibility in Nanoscale Drug Delivery. <i>ACS Applied Materials & Interfaces</i> , 2018 , 10, 31146-31157	9.5	67
82	Graphene-wrapped sulfur/metal organic framework-derived microporous carbon composite for lithium sulfur batteries. <i>APL Materials</i> , 2014 , 2, 124109	5.7	66

81	Structural chemistry, monoclinic-to-orthorhombic phase transition, and CO ₂ adsorption behavior of the small pore scandium terephthalate, Sc ₂ (O ₂ CC ₆ H ₄)CO ₂) ₃ , and its nitro- and amino-functionalized derivatives. <i>Inorganic Chemistry</i> , 2011 , 50, 10844-58	5.1	66
80	Adsorption of benzene, toluene, and xylenes on monolithic carbon aerogels from dry air flows. <i>Langmuir</i> , 2007 , 23, 10095-101	4	62
79	Targeted classification of metal-organic frameworks in the Cambridge structural database (CSD). <i>Chemical Science</i> , 2020 , 11, 8373-8387	9.4	61
78	Endocytosis Mechanism of Nano Metal-Organic Frameworks for Drug Delivery. <i>Advanced Healthcare Materials</i> , 2016 , 5, 2261-70	10.1	59
77	Mechanistic Investigation into the Selective Anticancer Cytotoxicity and Immune System Response of Surface-Functionalized, Dichloroacetate-Loaded, UiO-66 Nanoparticles. <i>ACS Applied Materials & Interfaces</i> , 2018 , 10, 5255-5268	9.5	56
76	Rare earth anthracenedicarboxylate metal-organic frameworks: slow relaxation of magnetization of Nd(3+), Gd(3+), Dy(3+), Er(3+) and Yb(3+) based materials. <i>Dalton Transactions</i> , 2016 , 45, 591-8	4.3	55
75	Design of a Functionalized Metal-Organic Framework System for Enhanced Targeted Delivery to Mitochondria. <i>Journal of the American Chemical Society</i> , 2020 , 142, 6661-6674	16.4	53
74	25 Years of Reticular Chemistry. <i>Angewandte Chemie - International Edition</i> , 2021 , 60, 23946-23974	16.4	50
73	Unusual adsorption behavior on metal-organic frameworks. <i>Langmuir</i> , 2010 , 26, 14694-9	4	48
72	Understanding excess uptake maxima for hydrogen adsorption isotherms in frameworks with rht topology. <i>Chemical Communications</i> , 2012 , 48, 10496-8	5.8	46
71	Trinuclear Cage-Like Zn(II) Macrocyclic Complexes: Enantiomeric Recognition and Gas Adsorption Properties. <i>Chemistry - A European Journal</i> , 2016 , 22, 598-609	4.8	45
70	Role of crystal size on swing-effect and adsorption induced structure transition of ZIF-8. <i>Dalton Transactions</i> , 2016 , 45, 6893-900	4.3	45
69	Carbon aerogels from gallic acid-resorcinol mixtures as adsorbents of benzene, toluene and xylenes from dry and wet air under dynamic conditions. <i>Carbon</i> , 2009 , 47, 463-469	10.4	44
68	Sol-Gel Synthesis of Robust Metal-Organic Frameworks for Nanoparticle Encapsulation. <i>Advanced Functional Materials</i> , 2018 , 28, 1705588	15.6	43
67	Discovery of an Optimal Porous Crystalline Material for the Capture of Chemical Warfare Agents. <i>Chemistry of Materials</i> , 2018 , 30, 4571-4579	9.6	43
66	Investigation of the terahertz vibrational modes of ZIF-8 and ZIF-90 with terahertz time-domain spectroscopy. <i>Chemical Communications</i> , 2015 , 51, 16037-40	5.8	39
65	Surface area and microporosity of carbon aerogels from gas adsorption and small- and wide-angle X-ray scattering measurements. <i>Journal of Physical Chemistry B</i> , 2006 , 110, 8681-8	3.4	39
64	Metal-Organic Framework Composites for Theragnostics and Drug Delivery Applications. <i>Biotechnology Journal</i> , 2021 , 16, e2000005	5.6	39

63	Permanent porosity derived from the self-assembly of highly luminescent molecular zinc carbonate nanoclusters. <i>Angewandte Chemie - International Edition</i> , 2013 , 52, 13414-8	16.4	37
62	Materials Informatics with PoreBlazer v4.0 and the CSD MOF Database. <i>Chemistry of Materials</i> , 2020 , 32, 9849-9867	9.6	37
61	Engineering new defective phases of UiO family metal-organic frameworks with water. <i>Journal of Materials Chemistry A</i> , 2019 , 7, 7459-7469	13	37
60	Tuning the Swing Effect by Chemical Functionalization of Zeolitic Imidazolate Frameworks. <i>Journal of the American Chemical Society</i> , 2018 , 140, 382-387	16.4	37
59	Structural dynamics of a metal-organic framework induced by CO migration in its non-uniform porous structure. <i>Nature Communications</i> , 2019 , 10, 999	17.4	36
58	Biocompatible, Crystalline, and Amorphous Bismuth-Based Metal-Organic Frameworks for Drug Delivery. <i>ACS Applied Materials & Interfaces</i> , 2020 , 12, 5633-5641	9.5	35
57	A Highly Porous Metal-Organic Framework System to Deliver Payloads for Gene Knockdown. <i>Chem</i> , 2019 , 5, 2926-2941	16.2	34
56	Structure-directing factors when introducing hydrogen bond functionality to metal-organic frameworks. <i>CrystEngComm</i> , 2015 , 17, 299-306	3.3	31
55	Tuning the Endocytosis Mechanism of Zr-Based Metal-Organic Frameworks through Linker Functionalization. <i>ACS Applied Materials & Interfaces</i> , 2017 , 9, 35516-35525	9.5	31
54	Modular structure of a robust microporous MOF based on Cu ₂ paddle-wheels with high CO ₂ selectivity. <i>Chemical Communications</i> , 2013 , 49, 11329-31	5.8	30
53	Controlling interpenetration through linker conformation in the modulated synthesis of Sc metal-organic frameworks. <i>Journal of Materials Chemistry A</i> , 2018 , 6, 1181-1187	13	30
52	Synthetic control of framework zinc purinate crystallisation and properties of a large pore, decorated, mixed-linker RHO-type ZIF. <i>Chemical Communications</i> , 2012 , 48, 6690-2	5.8	27
51	From synthesis to applications: Metal-organic frameworks for an environmentally sustainable future. <i>Current Opinion in Green and Sustainable Chemistry</i> , 2018 , 12, 47-56	7.9	27
50	Computational Screening of Metal Catecholates for Ammonia Capture in Metal-Organic Frameworks. <i>Industrial & Engineering Chemistry Research</i> , 2015 , 54, 3257-3267	3.9	26
49	First examples of metal-organic frameworks with the novel 3,3'-(1,2,4,5-tetrazine-3,6-diyl)dibenzoic spacer. Luminescence and adsorption properties. <i>Inorganic Chemistry</i> , 2013 , 52, 546-8	5.1	26
48	An open-access database and analysis tool for perovskite solar cells based on the FAIR data principles. <i>Nature Energy</i> , 2022 , 7, 107-115	62.3	26
47	Probing the Mechanochemistry of Metal-Organic Frameworks with Low-Frequency Vibrational Spectroscopy. <i>Journal of Physical Chemistry C</i> , 2018 , 122, 27442-27450	3.8	25
46	Enabling efficient exploration of metal-organic frameworks in the Cambridge Structural Database. <i>CrystEngComm</i> , 2020 , 22, 7152-7161	3.3	23

45	Enhanced gas sorption properties and unique behavior toward liquid water in a pillared-paddlewheel metal-organic framework transmetalated with Ni(II). <i>Inorganic Chemistry</i> , 2014 , 53, 10432-6	5.1	22
44	Tuning the target composition of amine-grafted CPO-27-Mg for capture of CO ₂ under post-combustion and air filtering conditions: a combined experimental and computational study. <i>Dalton Transactions</i> , 2015 , 44, 18970-82	4.3	20
43	Highly Active Anti-Diabetic Metal-Organic Framework. <i>Crystal Growth and Design</i> , 2016 , 16, 537-540	3.5	20
42	Novel 3D lanthanum oxalate metal-organic-framework: Synthetic, structural, luminescence and adsorption properties. <i>Polyhedron</i> , 2013 , 52, 315-320	2.7	20
41	Inter- and intra-primary-particle structure of monolithic carbon aerogels obtained with varying solvents. <i>Langmuir</i> , 2008 , 24, 2820-5	4	20
40	Nitro-functionalized Bis(pyrazolate) Metal-Organic Frameworks as Carbon Dioxide Capture Materials under Ambient Conditions. <i>Chemistry - A European Journal</i> , 2018 , 24, 13170-13180	4.8	19
39	Hydrogen uptake by {H[Mg(HCOO) ₃] ₂ NHMe ₂] _n and determination of its H ₂ adsorption sites through Monte Carlo simulations. <i>Langmuir</i> , 2011 , 27, 10124-31	4	19
38	Nanoporous carbon materials: Comparison between information obtained by SAXS and WAXS and by gas adsorption. <i>Carbon</i> , 2005 , 43, 3009-3012	10.4	16
37	Long lifetime photoluminescence emission of 3D cadmium metal-organic frameworks based on the 5-(4-pyridyl)tetrazole ligand. <i>Inorganica Chimica Acta</i> , 2015 , 427, 131-137	2.7	15
36	Formulation of Metal-Organic Framework-Based Drug Carriers by Controlled Coordination of Methoxy PEG Phosphate: Boosting Colloidal Stability and Redispersibility. <i>Journal of the American Chemical Society</i> , 2021 , 143, 13557-13572	16.4	15
35	"Explosive" synthesis of metal-formate frameworks for methane capture: an experimental and computational study. <i>Chemical Communications</i> , 2017 , 53, 11437-11440	5.8	14
34	Structural Elucidation of the Mechanism of Molecular Recognition in Chiral Crystalline Sponges. <i>Angewandte Chemie - International Edition</i> , 2020 , 59, 17600-17606	16.4	14
33	Computational Study of Propylene and Propane Binding in Metal-Organic Frameworks Containing Highly Exposed Cu ⁺ or Ag ⁺ Cations. <i>Journal of Physical Chemistry C</i> , 2014 , 118, 9086-9092	3.8	14
32	Advanced Monte Carlo simulations of the adsorption of chiral alcohols in a homochiral metal-organic framework. <i>AIChE Journal</i> , 2014 , 60, 2324-2334	3.6	13
31	Novel metal-organic frameworks based on 5-bromonicotinic acid: Multifunctional materials with H ₂ purification capabilities. <i>CrystEngComm</i> , 2012 , 14, 6390	3.3	13
30	How Reproducible are Surface Areas Calculated from the BET Equation?. <i>Advanced Materials</i> , 2020 , 32, 201502	24	12
29	Modulation of pore shape and adsorption selectivity by ligand functionalization in a series of box-like flexible metal-organic frameworks. <i>Journal of Materials Chemistry A</i> , 2018 , 6, 17409-17416	13	10
28	Screening Metal-Organic Frameworks for Dynamic CO/N ₂ Separation Using Complementary Adsorption Measurement Techniques. <i>Industrial & Engineering Chemistry Research</i> , 2019 , 58, 18336-18344	3.9	9

27	Towards a potential 4,4'-(1,2,4,5-tetrazine-3,6-diyl) dibenzoic spacer to construct metal-organic frameworks. <i>New Journal of Chemistry</i> , 2015 , 39, 6453-6458	3.6	9
26	Pore-Network Connectivity and Molecular Sieving of Normal and Isoalkanes in the Mesoporous Silica SBA-2. <i>Journal of Physical Chemistry C</i> , 2014 , 118, 10183-10190	3.8	9
25	Reverse Hierarchy of Alkane Adsorption in Metal-Organic Frameworks (MOFs) Revealed by Immersion Calorimetry. <i>Journal of Physical Chemistry C</i> , 2019 , 123, 11699-11706	3.8	8
24	Permanent Porosity Derived From the Self-Assembly of Highly Luminescent Molecular Zinc Carbonate Nanoclusters. <i>Angewandte Chemie</i> , 2013 , 125, 13656-13660	3.6	8
23	Structural Elucidation of the Mechanism of Molecular Recognition in Chiral Crystalline Sponges. <i>Angewandte Chemie</i> , 2020 , 132, 17753-17759	3.6	8
22	Advances in the Synthesis and Long-Term Protection of Zero-Valent Iron Nanoparticles. <i>Particle and Particle Systems Characterization</i> , 2018 , 35, 1800120	3.1	8
21	A comparison of copper and acid site zeolites for the production of nitric oxide for biomedical applications. <i>Dalton Transactions</i> , 2017 , 46, 3915-3920	4.3	7
20	Luminescence and Magnetic Properties of Two Three-Dimensional Terbium and Dysprosium MOFs Based on Azobenzene-4,4'-Dicarboxylic Linker. <i>Polymers</i> , 2016 , 8,	4.5	7
19	The launch of a freely accessible MOF CIF collection from the CSD. <i>Matter</i> , 2021 , 4, 1105-1106	12.7	6
18	Insights into the electric double-layer capacitance of two-dimensional electrically conductive metal-organic frameworks. <i>Journal of Materials Chemistry A</i> , 2021 , 9, 16006-16015	13	6
17	Identifying Differing Intracellular Cargo Release Mechanisms by Monitoring Drug Delivery from MOFs in Real Time. <i>Cell Reports Physical Science</i> , 2020 , 1, 100254	6.1	5
16	How Reproducible Are Surface Areas Calculated from the BET Equation?		5
15	Biological basis for novel mesothelioma therapies. <i>British Journal of Cancer</i> , 2021 , 125, 1039-1055	8.7	5
14	Structural heterogeneity and dynamics in flexible metal-organic frameworks. <i>Cell Reports Physical Science</i> , 2021 , 2, 100544	6.1	3
13	2D-cadmium MOF and gismondine-like zinc coordination network based on the N-(2-tetrazolethyl)-4'-glycine linker. <i>New Journal of Chemistry</i> , 2015 , 39, 3982-3986	3.6	2
12	Material Informatics with PoreBlazer v4.0 and CSD MOF Database		2
11	Wiz: A Web-Based Tool for Interactive Visualization of Big Data. <i>Patterns</i> , 2020 , 1, 100107	5.1	2
10	The development of a comprehensive toolbox based on multi-level, high-throughput screening of MOFs for CO/N separations. <i>Chemical Science</i> , 2021 , 12, 12068-12081	9.4	2

- 9 Insights into the Ultra-High Volumetric Capacity in a Robust Metal-Organic Framework for Efficient C₂H₂/CO₂ Separation. *Chemistry of Materials*, **2022**, 34, 2708-2716 9.6 2
- 8 Computational screening of functional groups for capture of toxic industrial chemicals in porous materials. *Physical Chemistry Chemical Physics*, **2017**, 19, 31766-31772 3.6 1
- 7 Lanthanide metal-organic frameworks for the fixation of CO₂ under aqueous-rich and mixed-gas conditions. *Journal of Materials Chemistry A*, **2022**, 10, 1442-1450 13 1
- 6 Metal-Organic Frameworks as Delivery Systems of Small Drugs and Biological Gases **2021**, 349-378 1
- 5 25 Jahre retikuläre Chemie. *Angewandte Chemie*, **2021**, 133, 24142 3.6 0
- 4 Computational techniques for characterisation of electrically conductive MOFs: quantum calculations and machine learning approaches. *Journal of Materials Chemistry C*, 7.1 0
- 3 Monolithic metal-organic frameworks for carbon dioxide separation. *Faraday Discussions*, **2021**, 231, 51-65 9.5 0
- 2 Molecular Sieving Properties of Nanoporous Mixed-Linker ZIF-62: Associated Structural Changes upon Gas Adsorption Application. *ACS Applied Nano Materials*, **2021**, 4, 3519-3528 5.6 0
- 1 Modulated self-assembly of an interpenetrated MIL-53 Sc metal-organic framework with excellent volumetric H₂ storage and working capacity. *Materials Today Chemistry*, **2022**, 24, 100887 6.2